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Development of Reliability Based Life Prediction Methods for Thermal and Environmental Barrier Coatings in Ceramic Matrix Composites

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FORWARD:

This report summarizes the technical work performed during the time period of June 2000 through October 2000 for the Order No. C-71140-K entitled "Development of Reliability Based Life Prediction Methods for Thermal And Environmental Barrier Coatings in Ceramic Matrix Composites." During this time period, literature survey related to the EBC/TBC (environmental barrier coating/thermal barrier coating) life models, failure mechanisms in EBC/TBC and the initial work plan for the proposed EBC/TBC life prediction methods development was developed as well as the finite element model for the thermal/stress analysis of the GRC developed EBC system was prepared. Technical report for these activities is given in the subsequent sections.

OBJECTIVE: The long term objective of the proposed work is to perform the research to model the structural behavior, cracking, crack propagation and develop reliability based life prediction of thermal barrier and environmental barrier coatings in ceramic matrix composites. However for the current funding period the scope is to:

(i) Perform literature survey and evaluate the current trend of research, technical direction, methods and computer codes used to assess the structural behavior characteristics, crack, crack propagation, life and uncertainties related to EBC/TBCs.
(ii) Develop a plan to approach the problem related to uncertainties, modeling, durability and life prediction and design of EBC/TBCs.
(iii) Discuss, report and concur on the approaches pursued and followed with the NASA Program Manager on a timely basis.
(iv) Document findings, benefits and shortcoming of different approaches in the form of a formal technical report.

BACKGROUND AND FAILURE/LIFE ISSUES RELATED TO EBC/TBC:

Computational model development research to predict behavior and failure of thermal barrier coatings (TBC) traces back to past three decades. However, a very little effort has been spent to develop life prediction models accounting for uncertainties in the governing variables. Current efforts in the Ultra Efficient Engine Technology (UEET) development program at the NASA Glenn Research Center (GRC) are focused not only on protecting components against severe thermal loads but also against the environmental effects such as moisture in the gas, debris, oxygen, etc. (references 1 and 2). The concept of protection against environmental effects is unique and novel under development at GRC. Current EBC/TBC material systems developed at NASA GRC are capable of delivering the expected performance up to 2400 °F temperature. However, new materials called environmental barrier coatings (EBC) are being developed to achieve desired thermal/environmental protection for components to operate at the gas temperature of 3000 °F, coating surface temperature of 2700 °F, and bond coat substrate interface temperature of at least 2400 °F with a desired life expectancy and assured reliability.

The current state-of-the-art EBC system under development in the UEET system consists of CMC (ceramic matrix composite) as substrate, silicon layer as a bond coat, a composite layer of mullite and BSAS (Barium Strontium Aluminum Silicate) and pure BSAS layer as EBC at the top. A pictorial representation of this system is shown in the figure 1.

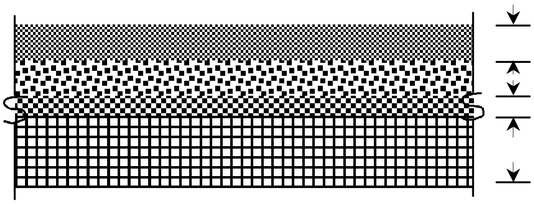

Figure 1. Typical Environmental Barrier Coating System under development in UEET Program

Silicon based ceramics are excellent candidates for high temperature application due to the slow formation of silicon oxide, however, there exist other problems related to the degradation and volatilization of the silica scale in the presence of water vapor, oxygen and alkali salts. Increasing the operating temperature range/magnitudes accelerate problems related to the oxidation of silicon, aluminum, BSAS, etc. as well as creep, degradation of the strength, properties of EBC/TBC during the thermal cyclic loads and gradients. These problems result into the sintering, creep deformation, cracking in the bond coat, formation of ridges and cavities, surface erosion, spallation of the coating as well as CMC, etc. ultimately affecting the durability of coatings. Spalling of the coating is induced by the bond coat oxidation accompanied by volumetric expansion during the high temperature exposure. Generally, the oxidation of the bond coat occurs due to the penetration of water vapor from combustion gases through the EBC/TBC and mullite layers.

Although, the mechanism of spallation has not yet been well understood, many speculative theories supported by some computational results have been proposed. Residual compressive stresses develop due to the differences in thermal expansion coefficients and stiffness of the bond coat. In addition, compressive stresses develop as a result of cooling in a thermal cycle and oxidation of bond coat accompanied by the volume change under constrained conditions at the interface. These conditions along with the stress relaxation during cooling cycle create normal stresses perpendicular to the interface at defect sites. Further growth of oxidation produces ridges and cavities at the interface layer. When normal stresses exceed the tensile strength, cracks form ultimately leading to the spallation due to volumetric changes. The geometry of interface and nature of the curvature (concave or convex) perpendicular to the interface affect spallation of coating significantly. In order to develop an effective coating system it is important to understand its behavior under these loading conditions and other environmental effects from the hot gases.

With the ever-increasing need for EBC/TBC in more critical applications, it is clear that life prediction has become an important issue to justify their full capability. It is also clear that modeling will be necessary for more efficient design of new EBC/TBC and for examination of the complex TBC failure mechanisms. Experimental investigations do lead to understanding its failures and mechanisms to a limited extent. However, it is important enough to quantify these effects and develop computational tools that can be used for material development and the EBC/TBC design purposes. It is to be noted here that EBC development is generic to NASA GRC and no literature is available on this subject outside of GRC sources. Therefore, the described approach focuses heavily on the GRC coating material development and design issues.

TASK I LITERATURE SURVEY:

Since the EBC is a GRC developed novel material development idea, it appears that research performed or pursued in the life prediction and cracking characteristic of the EBC is very limited. However, many approaches and methodologies pursued or implemented for TBC can be useful to the development of reliability based EBC/TBC life prediction and cracking characteristics.

Generally understood cracking behavior in the industry suggest that the following failure modes in the TBCs are of significant importance to the life/durability of the coatings as well as the coated components, reference 3:

Failure mode	Definition
Creep	Time dependent, thermally activated inelastic deformation of a material. The rate of creep increases as the temperature increases for constant stress.
High-Cycle fatigue	Microstructural damage mechanism that results from small stress amplitude cyclic loading, such as vibrations; failure will occur after a relatively large number of cycles.
Low-Cycle Fatigue	Microstructural damage mechanism that results from large stress amplitude cyclic loading, failure will occur after a relatively small number of cycles. Very abrupt thermal changes, such as from engine start and stop cycles, are the driving force for this failure mode.
High temperature Oxidation	Solid-gas chemical reaction that produces the oxide(s) of constituents within the solid. The rate of oxidation increases exponentially with temperature; certain oxides are slow growing and protective of the underlying substrate.
Hot Corrosion	Electrochemical reaction between substrate and molten salts, typically sodium and potassium sulfates. Two forms of hot corrosion are generally recognized: Type I (high-temperature), which typically occurs between temperatures of 820 °C and 920 °C, with a maximum of 870 °C, characterized by the buildup of a nonprotective oxide layer as oxidation and sulfidation destroy the metal substrate; and Type II (low-temperature), which typically occurs between temperatures of 590 °C and 820 °C, with a maximum of 700 °C, often exhibiting pitting.

Several other damage modes can also cause coating loss and accelerate the overall failure mechanism. These are:

(1) Mechanical distress to the coating, such as nicks and gouges, which is caused by objects ingested into the engine air stream.
(2) Solid-state diffusion of elements between coating and substrate, which can lead to the loss of critical elements from the coating and formation of undesirable phases in the substrate
(3) Spallation caused by differential thermal expansion between the coating and the substrate, which can lead to mechanical failure of the coating

(4) Rumpling of coatings as a result of creep

Cheng *et al*, reference 4, quantified the residual stresses in electron beam physical vapor deposited yttria stabilized zirconia thermal barrier coating system on a Pt-Al bond coat using the finite element analysis. Elasto-plastic analysis of the circular disk specimen modeled with actual interface surface with ridges and cavities showed significant areas of tensile stresses responsible to cracking. Some of the important conclusions of their study are listed below:

(i) Irregular interfaces lead to large tensile stresses in the thermally grown oxide (TGO) layer and cracking was observed where these stresses extend more than half way through TGO layer.
(ii) The stresses upon reheating that are missed in the elastic analysis were responsible for some of the observed cracking. Elastic analysis is not recommended for wavy surfaces.
(iii) Image processing can be used to obtain more precise geometry required to generate FEM models.
(iv) Use of actual interface geometry is more logical in FEM modeling than the commonly used sinusoidal geometries in the prediction of local stresses.

Brindley, reference 5, experimentally reviewed the effect of increasing the NiCrAlY bond coat oxidation resistance on TBC life. He showed that although the oxidation is a main driver, the significant difference in the coefficient of thermal expansion coefficient (CTE) and stress relaxation of the alloy in the bond coat has pronounced effect on the life whereas the elastic modulus of the alloy doe not. Stress relaxation of the bond coat for plasma sprayed coatings results in increase in the out-of-plane residual stresses at the bond coat peaks in bond coats that creep more and produces delamination of ceramic layer affecting the life.

DeMasi *et al,* reference 6, performed extensive experimental investigation of a two layer NiCrCoAlY TBC system to study its failure mechanisms and life model development. Important conclusions of their study are listed below:

(i) Spalling results from the progressive damage and oxidation is a significant driver. Bond crack oxidation was not conclusively shown to initiate the sub-critical cracks.
(ii) Increased coat thickness improves life.
(iii) Plasma sprayed ceramic exhibits nonlinear stress-strain response in uni-axial tension and compression, a strong creep response and stress sensitive fatigue behavior.
(iv) Life model that included Kevin walker constitutive model and oxide growth rate was developed and verified within a factor of ±3X.

Kokini *et al,* reference 7, have been studying TBC properties and its behavior under high thermal gradients and thermal cyclic loads. Their initial study (reference 7) focused on fracture mechanisms in TBC and effects of surface temperature as well as thermal gradients. For the CoCrAlY coating, the surface cracking is initiated by the stress relaxation resulting in the tensile stress during the cooling from high temperature to room temperature. Since the edge crack initiation has singular stresses, the stress criterion cannot be used although it shows both opening and shearing modes of cracks. The interface cracking is significantly different from the opening and shearing deformations with different energy release rates. Later they also studied the effects of laser heating, manufacturing process and thickness of coating on the cracking behavior of TBC, reference 8. Their experimental investigations revealed that the laser heating with sufficient energy could make the microstructure denser. With high energy and rapid heating, higher compressive stresses developed and decreased when cooled down to room temperature. Thus producing tensile stresses and more cracking. Another observation in relation to the manufacturing process is that the sintering and stress relaxation in a continuously manufactured thin ceramic layer lead to multiple surface cracks upon ambient cooling whereas in a thick layer it causes surface and interface cracks. Also, in the event that the stress field due to thermal heating is of a high intensity heating and it coincides with weakness within coating, it can cause delamination at that plane. These experimental investigations certainly help understand the response of TBCs to the high heat flux, manufacturing process transition thickness for interface delamination to multiple surface crack formation. However, computational simulation approaches are needed to understand behavior of EBC/TBCs in order to eliminate the necessity of a large number of experiments.

Lee, reference 1 and 2, identified the major issues related to the selection of EBC systems. These are:

- Ability to resist reaction with the aggressive environment
- Low oxygen permeability
- Coefficient of thermal expansion (CTE) must be close to that of the substrate material
- Ability maintain stable phase in thermal environment
- Chemical compatibility with the substrate material.

Based on the above requirements, Lee described the evolution of the mullite EBC system being developed at the NASA Glenn Research Center. Nonetheless, such a system still faces key durability issues such as through-thickness cracking in the mullite, weak bonding of mullite onto silicon-based ceramic and interface contamination at 2700 °F. It is still not known or verified computationally what causes through thickness cracks. However, it is strongly believed that these cracks allow the oxygen transportation that accelerates water vapor enhanced oxidation of the bond coat and eventual failure of the system. Additionally, the delamination of the bond coat, precipitation of second phase, such as residual amorphous mullite and alumina, in the mullite and the volumetric shrinkage reduce the durability of the EBC system.

Choules *et al,* reference 8, performed experimental studies on the effect of high heat flux on the thermal fracture of thermal barrier coatings on a steel base. Their study concentrated mainly on processing method (plasma spraying) such as interrupted and continuous spraying, coating thickness, and laser heating. The specimens tested are described in Table I and the specimen schematic is shown in Figure 2.

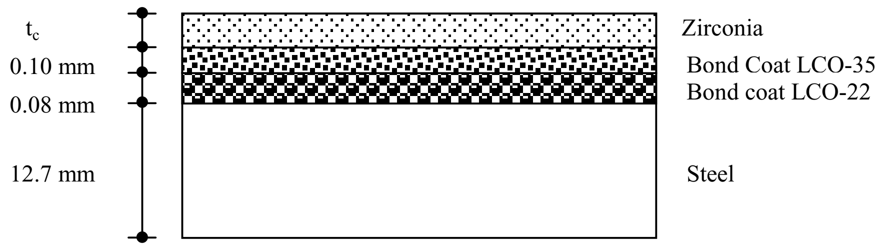

Figure 2. Thermal Barrier Coating for a steel substrate

TABLE I: TBC specimens tested to study the effect of processing methods (Choules *et al*)

Ceramic Layer		Measured substrate temperature (°C)			
		Preheat	Layer 1	Layer 2	
t_c mm	Plasma spray procedure	Bond coat	Final	Preheat	Final
0.66	Two pass preheat at 0.28mm above bond coat	Not measured	Not measured	Not measured	Not measured
0.76	Continuous	50	98	N/A	N/A
1.02	Two pass preheat at 0.28mm and 0.66mm above bond coat		Not measured	Not measured	Not measured
1.09	Continuous	53	101	N/A	N/A
1.09	Two pass preheat at 0.28mm above bond coat	50	98	54	93
1.09	Maximum preheat at 0.76 mm above bond coat	50	98	82	100

The effect of the 150 W and 200 W laser heating was studied in all specimens except 1.09 mm thick coating specimen. The heating was applied at an increment of 50 W until fracture was observed. The temperature gradients obtained was up to 1400 °C. Based on the observation the following conclusions were made by Choules *et al*:

(i) Laser heating of sufficient energy can change the material leading to denser microstructure.
(ii) Sintering and stress relaxation in a continuously manufactured thin ceramic layer lead to multiple surface cracking upon ambient cooling following laser heating.
(iii) Sintering and stress relaxation in a continuously manufactured thick ceramic layer lead to surface and interface cracking upon ambient cooling following laser heating.
(iv) If the stress field due to thermal heating is of sufficiently high, and it coincides with a plane of weakness within the coating, it is possible to cause delamination at that plane.

Based on the above literature, it is felt that the effect of processing, the coating thickness and time dependent behavior of the coating should be studied for the EBC system.

Andritschky *et al* (reference 9) studied the mechanics of delamination on the metal-based *thick* ceramic coatings. Delamination initiated by the transverse cracks caused by sintering process, thermal stresses and internal oxidation during prolonged exposure to the high temperatures were experimentally and computationally investigated. Coated samples were tested using four-point bending experiments to study the crack initiation along the substrate-coating interface and subsequent delamination due to tensile stresses. The residual stresses were obtained using the classical elastic theory by equating the average residual stress with the integrated analytically obtained stress distribution. The surface stress thus obtained matched with the observed stress using X-ray diffraction analysis. Force-displacement curves were used to determine the elastic properties of the coating. Analytical expressions based on the elastic theory were used to determine the Weibull distribution of the flexure stress. Since, it is difficult to identify the first micro crack and its corresponding stress, the experimentally observed deviation of the flexure stress at the first appearance of the crack was compared with that from the analytically obtained stress in order to determine the critical stress. Analytical equations using thin film theory and the effect of nearby cracks were used to obtain the stress distribution close to the fracture edge. However, for thick coatings linear FEM analysis was performed to obtain stress intensity factor (K_I and K_{II}). The FEM analysis superposed the analytically obtained residual stresses, which was approximate. FEM simulations were used in combination with the analytical classical fracture mechanics to compute stress intensity factors. However, their study concludes with the remark that the FEM analysis of the entire coating system can lead to better results due to the complexity of residual stresses, short cracks, multiple cracking, etc.

Teixeira *et al* (reference 10) quantified the residual stresses in the plasma sprayed TBCs induced by the processing and CTE mismatch. Computed residual stresses were compared with the experimental data and an acceptable was demonstrated. Studies under isothermal and cyclic heat treatment were conducted. Due to the CTE mismatch and/or thermal gradients, residual stresses develop in the coating leading to the adhesive (delamination of the interface) or cohesive failure (micro-cracking or spalling within the ceramic coating). Free edges exhibit large interfacial shear and axial stresses, which promote the micro cracking parallel and adjacent to the interface. During rapid thermal cycling the compressive stresses develop in the coating and causes the crack formation at the interface. Computational procedure involved 1D heat transfer with constant boundary conditions followed by the FE analysis.

Residual stresses in as deposited specimen as well as thermally cycled coatings were computed. The residual stresses were found not to be uniform through the thickness in the as deposited specimen and changed from tensile to compressive with increase in substrate temperature. The residual stresses were compressive at the interface diminishing toward the free surface in a linear manner. Difference between the computational and experimental results were attributed to the uncertainty in the physical properties of the plasma sprayed coating. The thinner coatings were found to have higher compressive residual stresses at the interface. Increase in the coating thickness showed surface stress changing from compressive to tensile.

During the rapid cycling the stresses in the oxide layer were assumed to be zero during the thermal growth. However, the compressive stresses develop in the oxide layer during the cooling cycle due to CTE mismatch with the substrate. The PVD (plasma vapor deposited) layer shows compressive stresses during the processing and increases after the thermal cycling. The PS (plasma sprayed) coating layer was in tensile state of stress at high temperatures and after thermal cycling due to stress relaxation as a result of micro cracking and creep phenomena. Thus, the residual stresses play a significant role in the life prediction model development.

Bao and Wang (reference 11) focused their study on multiple cracking in functionally graded materials (FGM). Multiple cracking is the most common phenomena in the coating systems, whether it is a TBC or an EBC. They studied the issue of multiple cracking from the fracture mechanics point of view by computing the crack driving force for the multiple cracks.

Cracking under mechanical load, thermal load and combined thermal and mechanical loads was studied. Linear elastic fracture mechanics coupled with finite element approach was used to compute the energy release rate of the cracks as determined by the coating degradation, crack length and crack density. In multiple cracking, the crack spacing usually attains saturation due to interaction of the neighboring cracks and relief of the tensile stresses in the coating. Their study, however, assumed the coating to be perfectly bonded to the homogeneous, isotropic metal substrate. This assumption fails to account for the debonding of coatings due to oxidation. Also, the plasticity of metal substrate as well as crack bridging mechanisms was neglected in their study. The functionally graded coating was divided into 100 layers and the equations for the properties of the functionally graded coating were derived as a function of the ration of the location from the top surface to the thickness of the coating. Equations for the energy release rates under different load conditions were derived. Energy release rates as function of the ratio of the crack length to the coating thickness as well as the crack density were computed and plotted for the mechanical, thermal and combined mechanical and thermal loads. Also the corresponding stress intensity factors were computed and plotted. Results showed that the FGM has higher hardness and oxidation resistance at the surface with much lower residual stresses and crack driving forces compared to that of pure ceramic coatings. The effect of mechanical loads on the crack driving force is found to be small. However, under thermal loads the effect on crack driving forces is significant.

Nusier *et al* (reference12) performed experimental and analytical investigation of the damage process in the thermal barrier coatings under different thermal cycle profiles. Attempts were made to describe progressive oxidation/damage evolution mechanistically. The diffusion equation using the Fike's Law was used to compute the oxide growth. However, no conclusions into the failure process, life and bond coat behavior were drawn.

One of the most important problems in the gas turbine engines that affect the TBC life is the erosion due to the foreign object impact (FOD) and moving gas under pressure at high speed. Understanding the phenomena from a mechanics viewpoint and the effect of the erosion rate is of equal significance for the life assessment. Wellman and Nicholls (reference 13) performed studies to explain the erosion process mechanism linked with the microstructure of the coatings. Their findings show that the velocity and radius of the object play a significant role in the surface cracking of the coating. Columnar structure of the coating has been shown to accommodate the strain. Three different patterns of microstructures in the columns of material were observed: (i) fern leaf dendrite type on the edges related mobility of atoms, (ii) striations fanning horizontally across the columns and (iii) numerous columnar crystallites that are closely packed. Number of cracked columns indicated brittle erosion mechanism and most of the cracks were perpendicular to the direction of column growth. The cracks propagated through the diameter of columns and tensile stresses were responsible for it. Also, cracks did not propagate into the neighboring columns and not more than five columns adjacent to the cracked one were found cracked. Observations showed no correlation with the column diameter and the depth at which crack occurs. Also, no existence of shear cracks was observed. Variations in the Young's modulus and Poisson's ratio of the target have very little effect on the contact radius. The depth at which cracking occurs was direct function of the impacting particle radius and velocity. Near surface cracking and the dendrite initiated cracking was most predominant erosion mechanism. All the observations were experimental and were not supported by the computational methods.

TASK II PROPOSED APPROACH AND WORK PLAN:

The proposed future plan for the Life Prediction Methods development for the environmental barrier coatings (EBC)/ thermal barrier coatings (TBC) system for ceramic matrix composites (CMC) being developed at GRC is physics based, compliments the material development process, and lead to the final state-of-the-art computationally efficient design tool development. Following paragraphs describes salient features of the approach.

II.1 ISSUES RELATED TO EBC/TBC IN UEET PROGRAM:

Critical issues (reference 1 and 2) that relate to the EBC/TBC system development under the UEET program are: (i) Chemical incompatibility between the silica and Si based ceramics that result into the pore development in the reaction zone and interface delamination, (ii) volatilization of the silica under high temperature in the presence of moisture and oxygen, (iii) mismatch between the coefficient of thermal expansions of substrate and coating resulting into the residual stresses and surface cracks, (iv) initial flaws due to nicks and gouges as results of foreign object impacts, (v) through and surface crack development in the coating due to thermo mechanical loads, (vi) spalling under thermal cyclic, and (vii) sintering causing volumetric changes that result into the mudflat cracks.

II.2 PERCEIVED PRELIMINARY FAILURE MECHANISM IN EBC/TBC:

It is important to understand the real physical behavior of the EBC/TBC coating system under thermo-mechanical cyclic loads in order to understand the issues described above. Based on the personal discussions with Lee (references 1 and 2), the perceived preliminary failure mechanism has been described herein. During the manufacturing process, several passes of the coating are applied under prescribed thermal conditions. Cooling and heating involved in the process result into the residual thermal stresses built up. After formation of the coating, micro level cracks in the surface as well as through the thickness have been observed. Additionally, the cracks in the surface form due to the mechanical distress to the coating, nicks and gouges caused by objects ingested into the engine air stream. Also, thermal gradient between substrate and coating develops under the operating conditions of thermal shocks and thermal cycles mainly due to the difference in the thermal conductivity and requirement of maintaining substrate temperature within certain level.. Under the cyclic nature of the thermal load and mismatch in the thermal expansion coefficients of the coating, mullite, silica and substrate, residual stresses develop as well as stress relaxation occurs in these layers. These conditions aggravate or accelerate the crack formation and growth in the coating system layers.

Once, the cracks in the coating system forms and grows as the components undergo increased operation, the moisture, oxygen and alkali slats present in the gas penetrates to the silica layer. Under high temperature conditions and presence of these agents, the silica oxidation starts and formation of the silicon oxide begins/continues. Continued formation of the SiO_2 results into the volumetric changes involving shrinkage and swelling. Furthermore, the oxidation results into sintering and spalling of the coating. Volumetric changes accompanied by the cyclic nature of stresses, the crack formation, growth and silica oxidation continues until the system fails.

II.3 PROPOSED WORK PLAN OBJECTIVE:

Having described the issues and perceived failure mechanism in the EBC/TBC system, the objectives of the proposed work plan are:

(i) Develop a generic reliability based EBC/TBC life prediction methodology
(ii) Capture uncertainties associated with the EBC/TBC life
(iii) Identify and quantify the sensitivity of variables governing the EBC/TBC life
(iv) Quantify the reliability of EBC/TBC life
(v) Develop generic and general-purpose computational design tool for EBC/TBC life prediction.

II.4 PROPOSED APPROACH PLAN:

The proposed approach plan is divided into three main categories: (i) Heat transfer analysis, (ii) Physics based deterministic life prediction model development, (iii) reliability based life prediction method development.

II.4.1 Heat transfer (HT) analysis: A transient heat transfer analysis of the EBC system shall be performed to calibrate the experimentally obtained thermal properties, compute non-measurable thermal properties, estimate temperature gradients, and develop thermal design guidance for the EBC/TBC system for the desired substrate, surface and gas temperatures. Computational 2-D and 3-D models to perform the heat transfer analysis have already been prepared and shown in Figures 3 and 4 respectively. Following are the 2-D FEM model details:

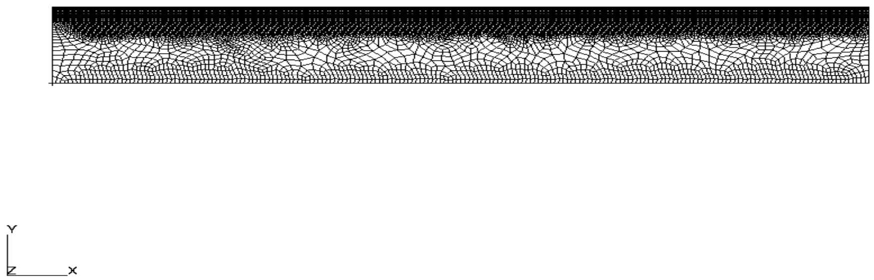

Figure 3a. 2D Finite element model for the EBC material system.

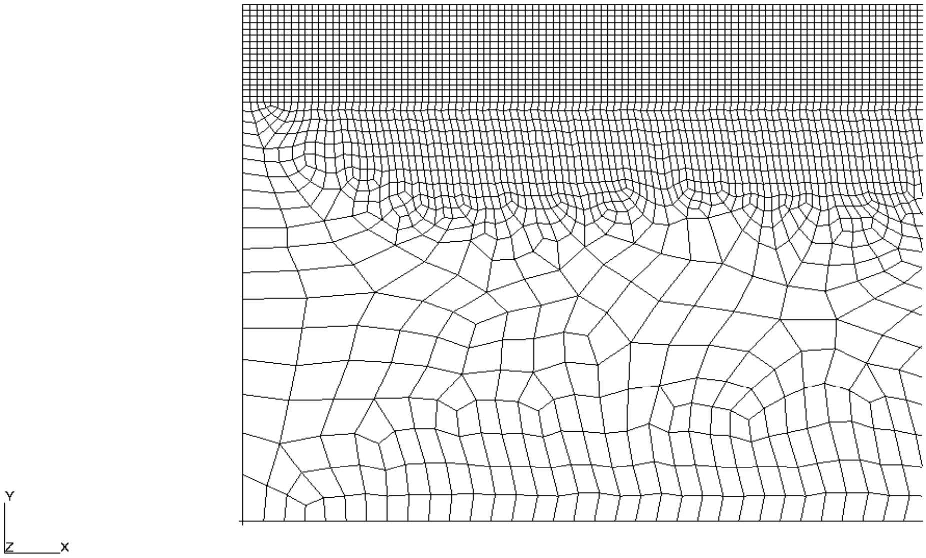

Figure 3b. Portion of the 2D finite element model at the edge

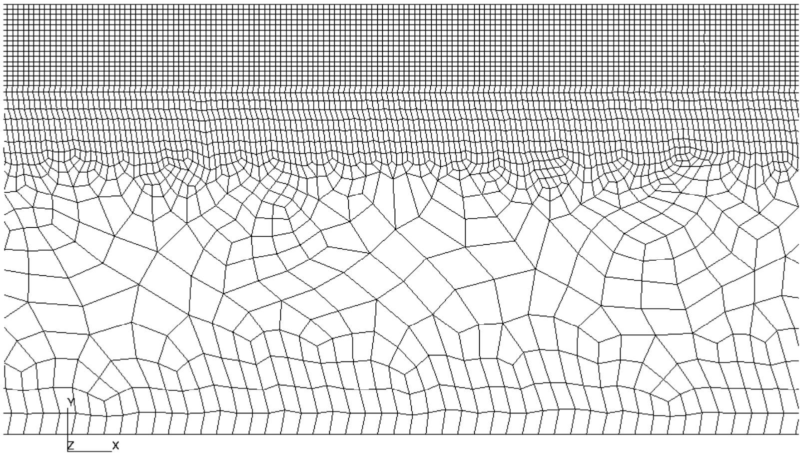

Figure 3c. Portion of the 2D finite element model in the middle

Number of Nodes:	17272
Element type:	2D Shell
Number of Elements:	16837

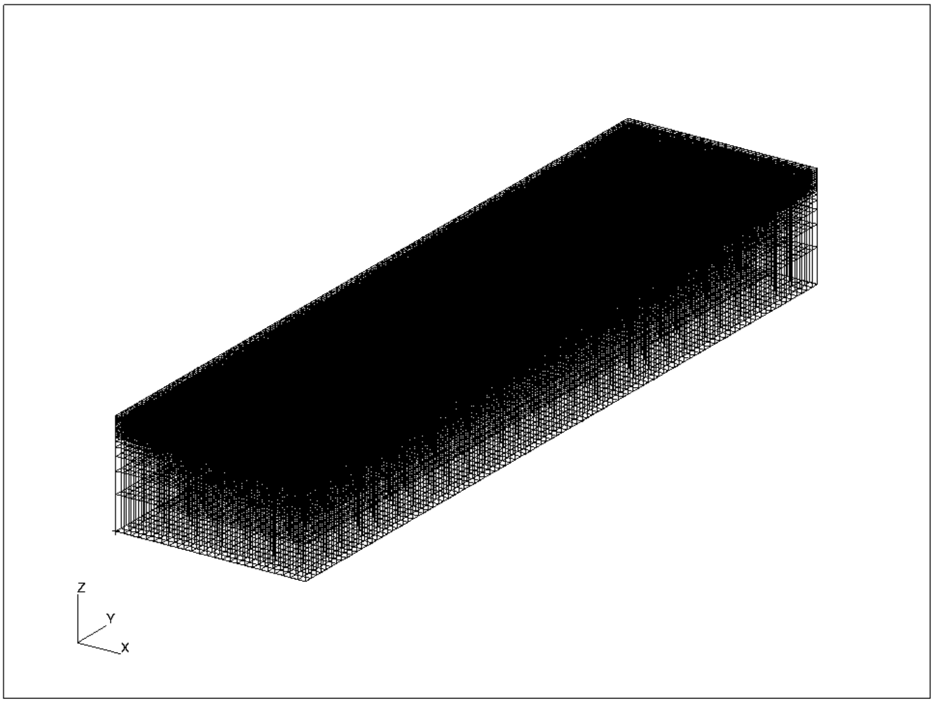

Figure 4a. 3-D Finite element model

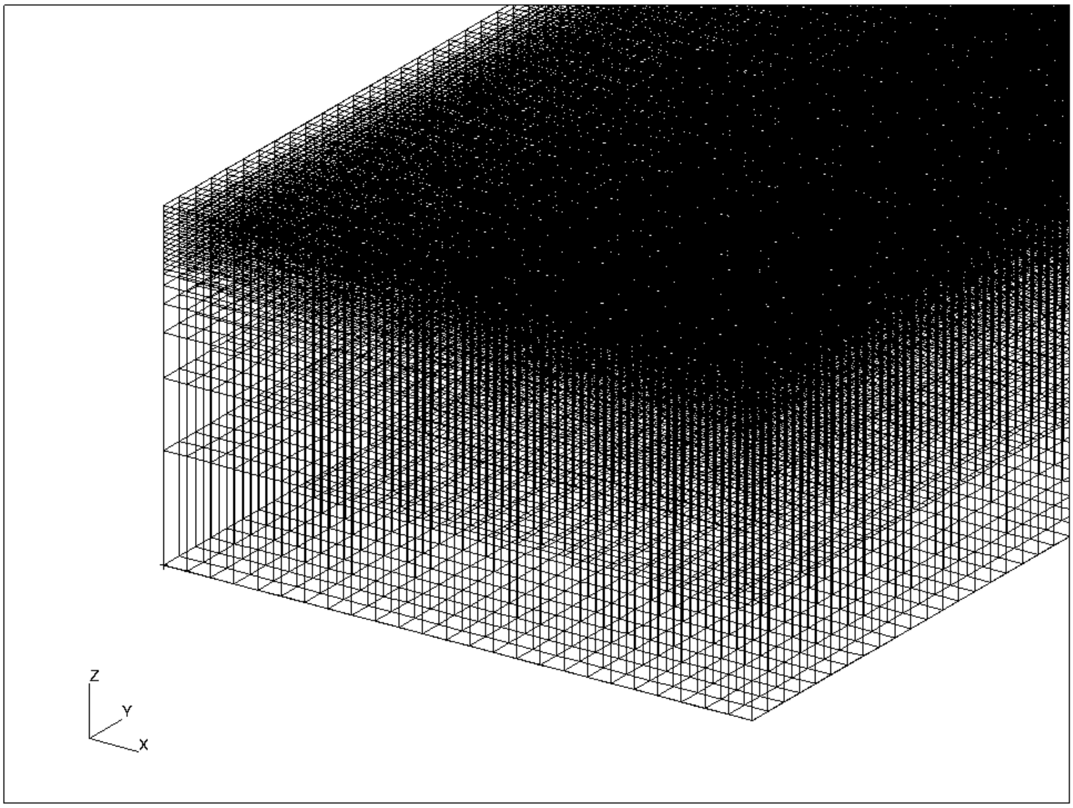

Figure 4b. Portion of the 3-D finite element model

The purpose of the 2-D model development and analysis is for preliminary quick estimation of the thermal gradients, experimental data calibration and compute non-measurable properties. Purpose the 3-D model is to obtain refined results related to the 3-D state of stress related to failures in EBC/TBC. 2-D analysis allows modeling the conduction effects only. Results of the preliminary 2-D HT analysis are shown in Figure 5. The results show that the thermal gradient between the top of the substrate surface and coating top surface is about 100 °F which shows that the thermal conductivity of the EBC is quite low.

In order to understand the thermal behavior further, it was felt necessary to include the convection effects in the analysis. To evaluate the convection effects, a 3D finite element model using the 3D solid element for the same EBC system was prepared which is also intended for use to perform the stress analysis. The size of the 3D model is also comparable to the 2D model and is expected to run efficiently for both thermal and stress analyses. Preliminary film coefficient of the coating surface for the combustor liner at different locations obtained from the NASA Program Manager was used. Average value of the film coefficient was used in the analysis. First assessment of the 3-D HT analysis is shown in Figure 6. Results are quite similar to those obtained in the 2-D analysis. Further investigation is needed and shall be continued in the future work. However, the purpose of a 3-D model development was also to define the failure criteria more effectively, understand failure mechanism and model uncertainties related to the geometry as well as crack density in a reasonable manner, which is a part of the proposed future work.

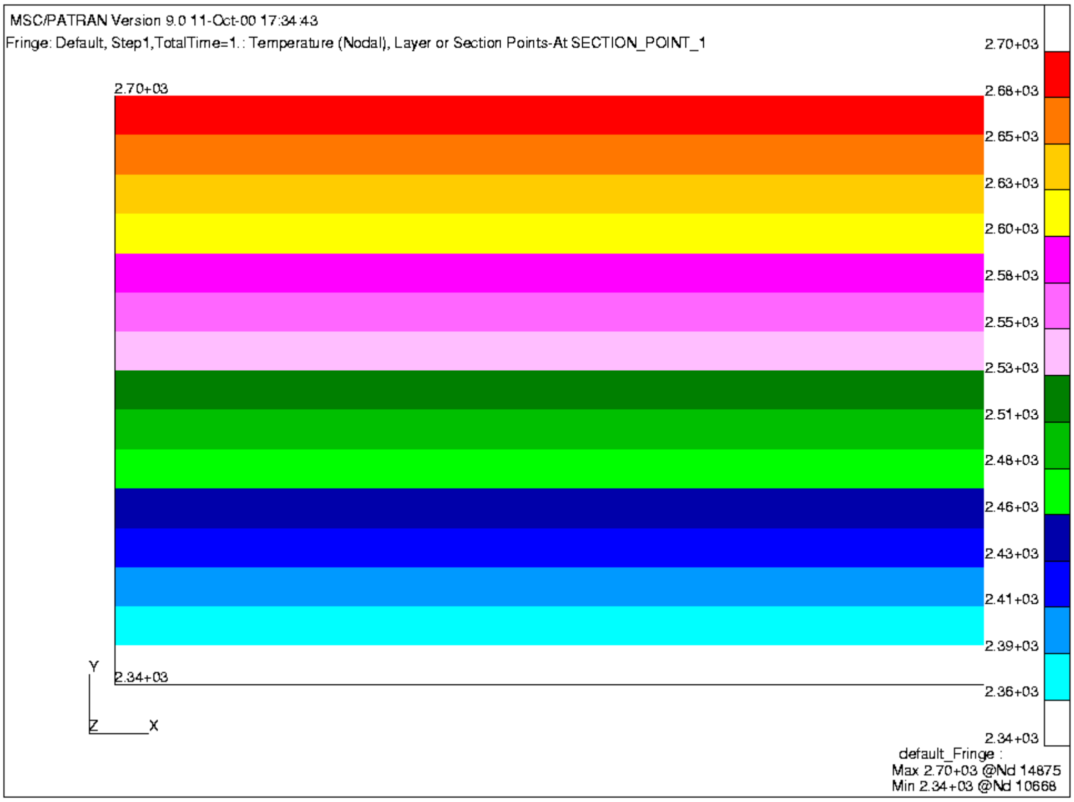

Figure 5. Temperature distribution in the EBC coating system 2-D analysis
(Gas Temp = 3400 °F)

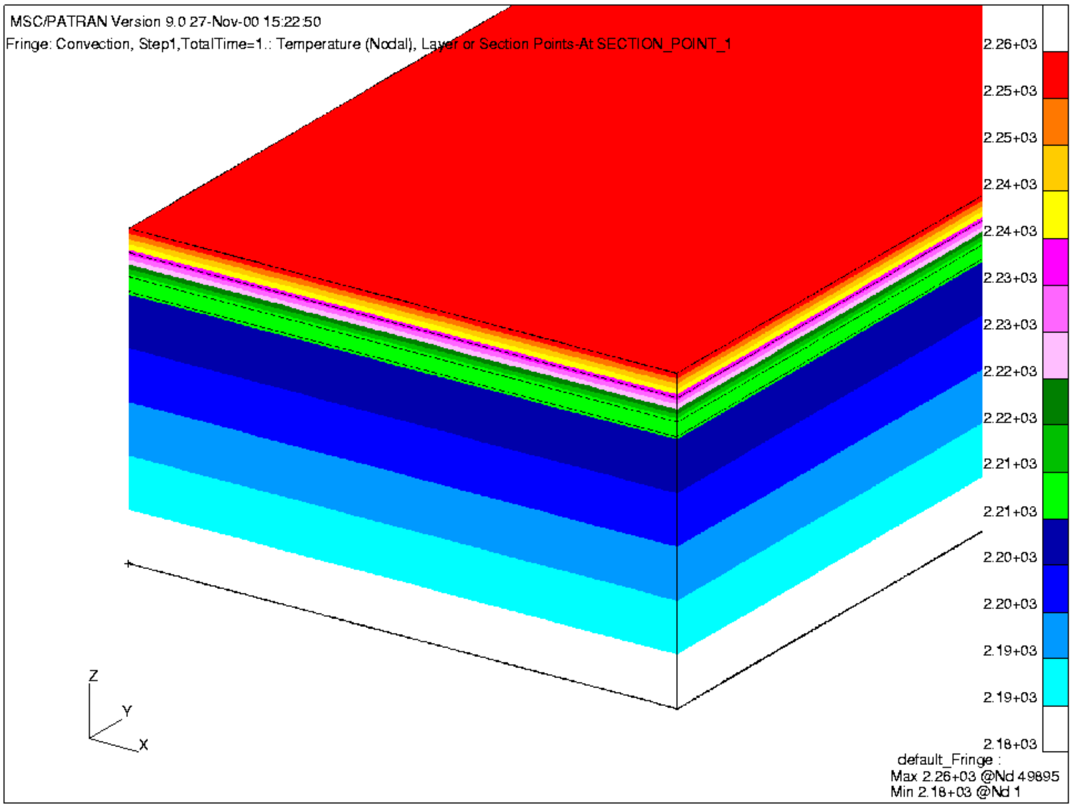

Figure 6. Temperature distribution in the coating system 3-D analysis
(Gas temperature = 3100 °F)

As a part of the future work on HT analysis, measured thermal properties of coatings, bond coat, substrate, such as thermal conductivity, film coefficients, etc. shall be used in the transient cyclic heat transfer analysis to compute the temperature distribution across the EBC/TBC system and compared with the measured surface temperatures or other data. Comparison shall be done to calibrate the computational process. A matrix of different analyses based on the experimental plans shall be prepared in order to achieve the objective of calibration. Further discussion about the analysis matrix and heat transfer analysis is documented with that of stress analysis.

II.4.2 Physics based deterministic life prediction method development:

Life prediction methods development of EBC/TBC system is a formidable task. In order to assess the life of coatings, a reasonably accurate stress analysis and long term behavior of the coating while modeling the real physical aspects need to be simulated. Therefore, a transient analysis that couples the heat transfer and stress analysis in a probabilistic sense is proposed as a core of the approach. To achieve this objective, the approach planned here is physics based. The outline of the approach is given in Figure 7.

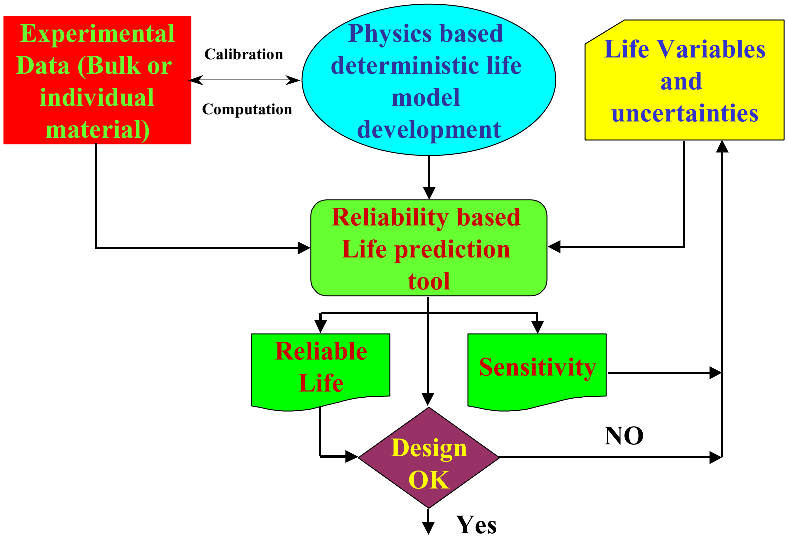

Figure 7. Proposed EBC/TBC life development approach outline

The proposed approach aims at computing the functional life of the coating and not till its failure. Since the design procedures aims mainly at the functional behavior of the coating and also the fact that the continued life after the exposure of the substrate to the thermal effects of the gas is very little, simulation of the complete failure of the coating is not needed. Therefore, the approach proposed herein, simulates the failures to the functional level only and the meaning of the word failure be taken in this context hereinafter. The physics based approach aims at simulating the following:

(1) Residual stress development due to the coefficient of thermal expansion (CTE) mismatch between substrate, bond coat, mullite and coating
(2) Penetration of the moisture and oxygen to the bond coat through the existing pores and cracks (Figure 8)
(3) Oxide growth formation
(4) Shrinkage and sintering effects
(5) Material degradation especially that of the bond coat
(6) Failure of coating

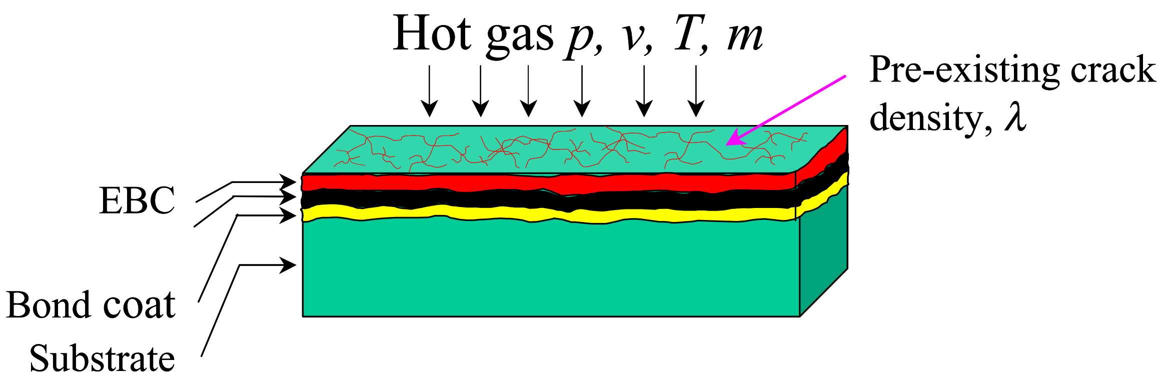

Figure 8. Bond coat degradation mechanism

Following the above simulation requirement, the life prediction approach is divided into different parts: (a) Crack formation phenomena and oxidation rate kinetics modeling, (c) FEM application, and (d) Life prediction model development.

II.4.2.1 Crack formation phenomena and oxidation rate kinetics modeling:

As explained in the section II.2, the cracks/pores in the coating surface as well as through the thickness exist due to the manufacturing process, nicks and gouges due to the ingestion of foreign objects. Even under the controlled conditions in the laboratory, these cracks have been found and its density has been measured. The moisture, oxygen and alkali salts present in the gas penetrate through these cracks and initiates/accelerates the oxidation/volatilization of the silicon bond coat (Figure 8). Obviously, the rate at which oxidation occurs depends upon the amount of moisture, oxygen, alkali salts present in the gas, velocity, pressure, and temperature of the gas as well as the crack density. Oxidation of the silicon results into the volumetric change as well as its structural property degradation. Owing to these conditions together with the heating and cooling under cyclic thermo/mechanical loads resulting into the residual stresses due to CTE mismatch, the bond coat undergoes the volumetric (scale thickness) changes. Due to the volumetric changes, the scale thickness changes and internal pressure develops, which becomes an additional load on the coating system. The combined effect of these changes entails into the growth of the existing cracks and formation of new cracks and hence the crack density as well as the moisture, oxygen penetration rates. A continued phenomenon of silicon oxidation degrades the bond with the substrate and interface cracks also develop as well as the substrate gains more exposure to the hot gas which ultimately fails.

In order to develop a physical model of the above phenomena, a diffusion equation using the Fick's Law can be used to describe the progressive oxidation/damage evolution. Equations for the moisture and oxygen penetration rate as a function of crack density; pressure, velocity, temperature, moisture and oxygen content of the gas can be developed using the analytical and experimental methods. Simplified tests can be developed and performed to achieve this objective. Although these equations turns out to be empirical in nature, the effectiveness of their application can be realized using the probabilistic approaches discussed later in this report.

Once, the governing rules/law for the oxidation rate determination are cast into the diffusion equation, the oxidation rate can be easily tied to the Arrhenius law to compute the change in scale thickness/spallation using the activation energy and gas law. Robinson and Smialek, *et al* (References 14 and 15) have developed relationship between the scale thickness and oxidation rate when it is completely exposed to the gas. Their ideas and methodology can be modified for the purpose of EBC/TBC bond coat oxidation and spallation simulation.

II.4.2.2 FEM APPLICATION:

Upon developing the physics based crack formation and oxidation kinetic model, the next important step in the approach development is to implement them in the finite element analysis. Analytical implementation involves preparing the mesh, material properties, material degradation model, and failure criteria definition. Determining time dependent materials properties, both thermal and structural, experimentally is a challenging task. Therefore, from an engineering point of view, it is necessary to devise a series of computational virtual experiments using the available individual and bulk properties to obtain required material properties for the life prediction development. Such computational experiments may require judiciously and logically ascertained trial and error process. Validity and verification of these virtual experiments shall be confirmed through the comparison with the simulated results with those measured in the laboratory at macro or bulk level.

Thermal and structural properties of each individual coating system constituents, estimated from the laboratory and computational experiments, can be used to perform the coupled transient HT and stress/failure analysis of the EBC/TBC system. The actual physical behavior implementation requires using the adaptive meshing technique in the transient analysis to account for the volumetric change (scale thickness), pressure exerted due to it, change in the crack density and moisture penetration rate, and material degradation. Commercial finite element software packages such as ABAQUS or MARC can be used to achieve adaptive meshing implementation. Simple functional failure criteria shall be developed that addresses the individual material failure, delamination of the coating system layers, etc. Additionally, the 3-D analysis is aimed at simulating the effect of the actual interface geometry that creates the ridges and valleys resulting into the sites with stress concentrations and eminent failure or its initiation.

Established and reliable analytical approach described above provides the hours in the number of cycles/hours of operation. The next step is to develop a life prediction model for the EBC/TBC system. An analyses matrix reflecting controlling variables will be prepared to aid the process of life prediction model development. Results of several analyses runs while controlling and varying the governing design parameters/variables can be correlated with the available experimental data and deterministic life prediction model/equations can be developed. Although the developed model may be based on the limited experimental data, the effectiveness of the model will become attractive with the inclusion of uncertainty simulation in the life. Also, the process enables the design of thick EBC/TBC system.

II.4.2.3 Reliability based EBC/TBC Life Prediction Method Development:

Due to the variations in the manufacturing and application processes, chemical conditions, thickness, initial crack density, interface geometry, material properties of the coating system, the behavioral characteristics of the EBC/TBC vary considerably. Additionally, the inherent uncertainties in the gas temperature, pressure, velocity, moisture, oxygen and alkali salt contents, thermal shocks during the engine startup, etc. affect the performance of the coating. Continued exposure in combustion environment with these uncertainties can lead to significant variation in the actual life.

Deterministic understanding of the structural characteristics of EBC/TBC from the life and durability point of view becomes a complicated task due to the above-described uncertainties. Initial survey of the literature suggests that very little and perhaps no research effort using the probabilistic approaches is going on at present in the government, industry as well as academia. Also, the existing deterministic research has not produced results to achieve desired objective of predicting EBC/TBC life with assured reliability.

Understanding the issues, difficulties in developing deterministic approaches and uncertainties in the design variables, it is proposed to extend the method described in Task II.4.2.2 in a probabilistic domain. Probabilistic approach enables the simulation of uncertainties, and quantifies the sensitivity of the basic design variables to the reliability of the life. Majority of the probabilistic approaches are random variable based which are applicable to static and linear problems. EBC/TBC life model development is a time domain problem and involves material non-linearity with time. Therefore, a stochastic process based approach that integrates thermal, structural and non-linear behavior uncertainties to simulate the long-term behavior shall be developed/adopted.

Stochastic process approach deals with the uncertainties that are functions of time as well. The value of variable, X changes with time, t, which depends on its value at previous times and therefore has a probability distribution at each instance of time. The joint probability functions of X(t) at different times and given by

$$F_{\{x\}}(x_1, x_2; t_1, t_2) = P(X(t_1) \le x_1) \cap X(t_2) \le x_2))$$

A stochastic process is characterized by its mean and auto-correlation function given in the equation form as

$$\mu_x(t) = E[X(t)] = \int_{-\infty}^{\infty} x f_x(x;t)dx$$

$$R_{xx}(t_1, t_2) = E[X(t_1)X(t_2)] = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x_1 x_2 f_x(x_1, x_2; t_1, t_2)dx_1 dx_2$$

A stochastic process can be decomposed into its characteristic variables and characteristic functions using Karhunen-Loeve, reference 16, expansion procedure, which can be used directly in the probabilistic analysis. Markov chain or barrier crossing analysis (Figure 9) approaches (reference 17) can be used to compute the probability of exceeding the certain value of responses, which is life in the EBC/TBC work, as well as the frequency of exceeding it in a given time interval t. Additionally reliability methods such as time domain second order reliability methods for multiple failure modes can be used to compute reliability of the coating (reference18, using the following equations).

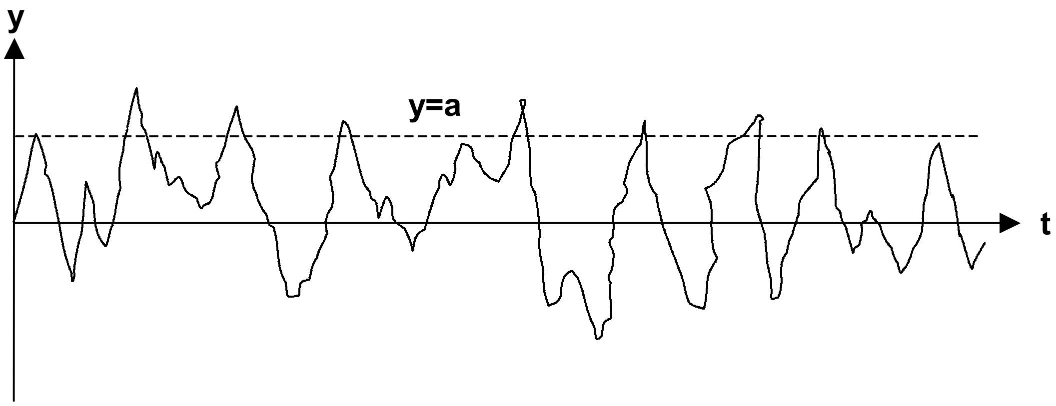

Figure 9a. Time history of response y and a barrier at y=a

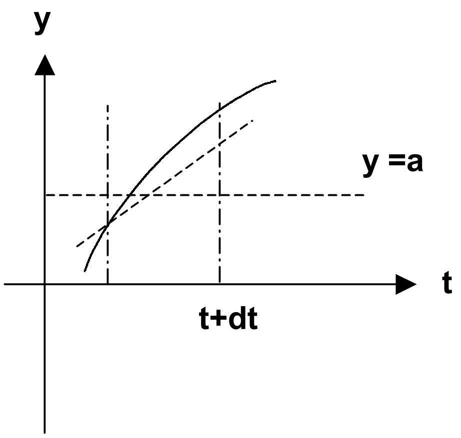

Figure 9b. Condition for positive slope crossing of barrier at y=a

At time t, the cumulative distribution function (CDF) F, the mean E[R(t)], and the standard deviation σ for any structural response R(t) (displacement, stress, strain, etc.) can be defined as

$$F_{R(t)}(z_i) = \Phi(-\beta_i^t) \qquad i = 1,...k$$

$$E[R(t)] = \overline{R}(t) = \sum_{i=1}^{k} z_i f_R(z_i)\Delta z$$

and

$$\sigma_{R(t)} = \sqrt{\sum_{i=1}^{k} \left[z_i - \overline{R}(t)\right]^2 f_R(z_i)\Delta z}$$

where Φ is the standard normal cumulative distribution function; β is the first-order-second-moment (FORM) reliability index, k is the number of discretizations, and $f_{R(t)}$ is the probability density function (pdf) of R(t) (reference 18, Lind et al., 1985)

Define X(t) (stress, strain, displacement, etc.) as the random process, and let R_1 and R_2 be any two responses from X(t), then the joint CDF F_{R1R2} is given by

$$F_{R_1R_2}(z_i, y_j) = \Phi(-\beta_i)\Phi(\beta_j) + \int_0^{\rho_{ij}} \phi(-\beta_i, \beta_j; u)du \qquad i = 1,...,k \quad and \quad j = 1,...,l$$

where (z_i,y_j) are any pair of realizations, ρ_{ij} is the correlation between realizations. Let $R_1=X(t_1)$ and $R_2=X(t_2)$, the autocorrelation function of the process X(t) is

$$\rho(t_1, t_2) = \frac{\sum\sum\left[z_i - \overline{X}(t_1)\right]\left[y_j - \overline{X}(t_2)\right] f_{x(t_1)x(t_2)}(z_i, y_j)\Delta z\Delta y}{\sigma_{x(t_1)}\sigma_{x(t_2)}}$$

where $f_{x(t1)x(t2)}$ is the joint pdf of $X(t_1)$ and $X(t_2)$.

The mean rate at which a random process X(t) (x can be stress, strain, displacement, etc.) crosses a random threshold level $\xi(t)$ (which can be the failure criteria) is given by

$$v_{\xi}(t)=\int_{0}^{\infty} f_{x(t)\dot{x}(t)}[\xi(t),\dot{x}(t)]\,\dot{x}\,d\,\dot{x}$$

Once, the crossing rates are determined the algorithm can be tied with the durability analysis to compute reliability of the structure for a desired life.

As a byproduct of the probabilistic analysis, sensitivity of the design variables can be quantified, which is useful to improve the design. As mentioned earlier in the physics based methods development, the sensitivity information can be used to compute the non-measurable properties of the coating system as well as the material development process. Using the probabilistic analysis results, the guidelines for the maintenance and inspection intervals can be developed.

Typical results that will be computed for the reliability based EBC/TBC life development effort is e.g. reliability based thickness of the coating system versus life curve (Figure 10), thermal gradient versus life for a given coating system, etc.

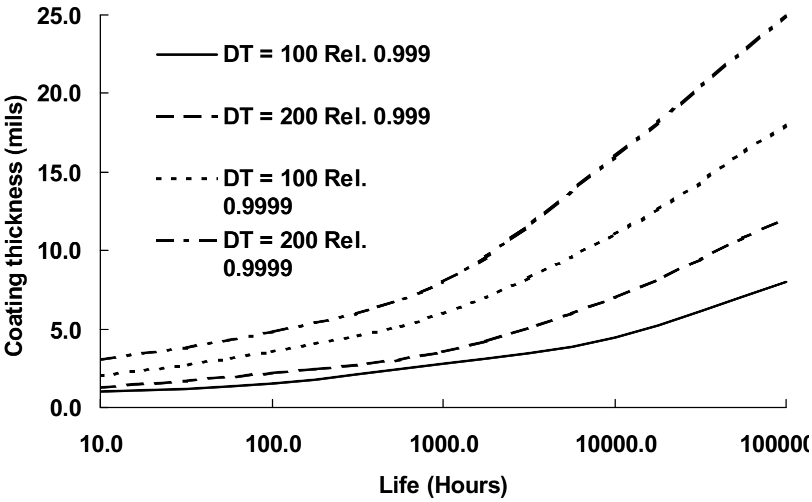

Figure 10. Typical EBC/TBC reliability based life curve results

II.5 Design tools development and objective:

The ultimate objective of the proposed effort is not to just develop the EBC/TBC life prediction methodology, but also to develop a software tool to design the barrier coating systems. The objectives of the design software tool are: (i) simple to use that can be linked with any commercial FEM package, (ii) easy to identify input parameters, (iii) enables the user to configure a coating systems configuration, (iv) provide design improvement guidelines, and (v) develop reliability based life curves.

TASK III PROGRAM MANAGEMENT:

Discussions on progress and technical thoughts, approaches and plan were held regularly with Dr. Dave Brewer, Dr. Murthy, Dr. Kang Lee of NASA GRC as well as other technical personnel during the course of the work. Monthly technical progress and financial reports were submitted to the NASA Program Manager. Also, an abstract titled, “Current issues related to life prediction of environmental barrier coatings in ceramic matrix composites” was submitted for the possible publication in the upcoming AIAA SDM Conference in Seattle, WA to be held on 16 Apr 2001 to 19 April 2001.

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13. ABSTRACT *(Maximum 200 words)*

This report summarizes the technical work performed during the time period of June to October 2000 for the Order No. C–71140–K entitled “Development of reliability based life prediction methods for thermal and environmental barrier coatings in ceramic matrix composites.” During this time period, literature survey related to the EBC/TBC (environmental barrier coating/thermal barrier coating) life models, failure mechanisms in EBC/TBC, and the initial work plan for the proposed EBC/TBC life prediction methods development was developed as well as the finite element model for the thermal/stress analysis of the GRC-developed EBC system was prepared. Technical report for these activities is given in the subsequent sections.

14. SUBJECT TERMS

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